

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.81e-09 mmHg

Global applicability domain: Inside

Local applicability domain index: 2.50e-01

Confidence level: 3.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,4,5-Trimethylphenol</div> <div>Measured: 7.50e-08</div> <div>Predicted: 1.72e-02</div>	<div>Image not found</div> <div>Dibenzofuran, 1,2,3,4,8-pentachloro-</div> <div>Measured: 2.84e-11</div> <div>Predicted: 2.10e-09</div>	<div>Image not found</div> <div>Hexythiazox</div> <div>Measured: 1.01e-08</div> <div>Predicted: 2.42e-08</div>
<div>Image not found</div> <div>Naphthalene, 1,2,4,7-tetrachloro-</div> <div>Measured: 3.45e-10</div> <div>Predicted: 1.23e-05</div>	<div>Image not found</div> <div>2-Dodecanone</div> <div>Measured: 6.67e-07</div> <div>Predicted: 2.01e-02</div>	